The Material Editor

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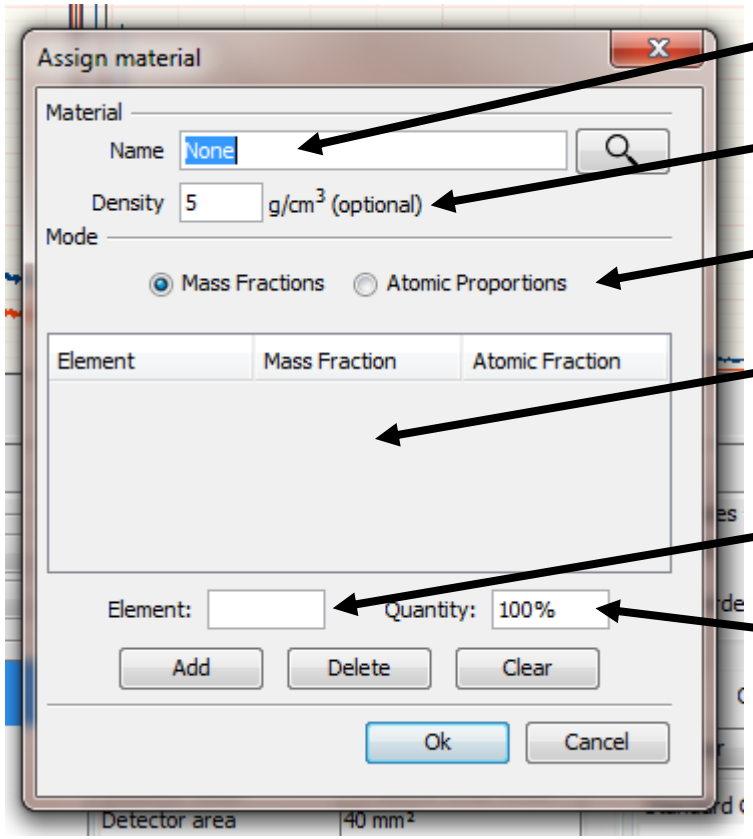
The tedious way…



A unique human friendly name

The density is required for Monte Carlo simulations

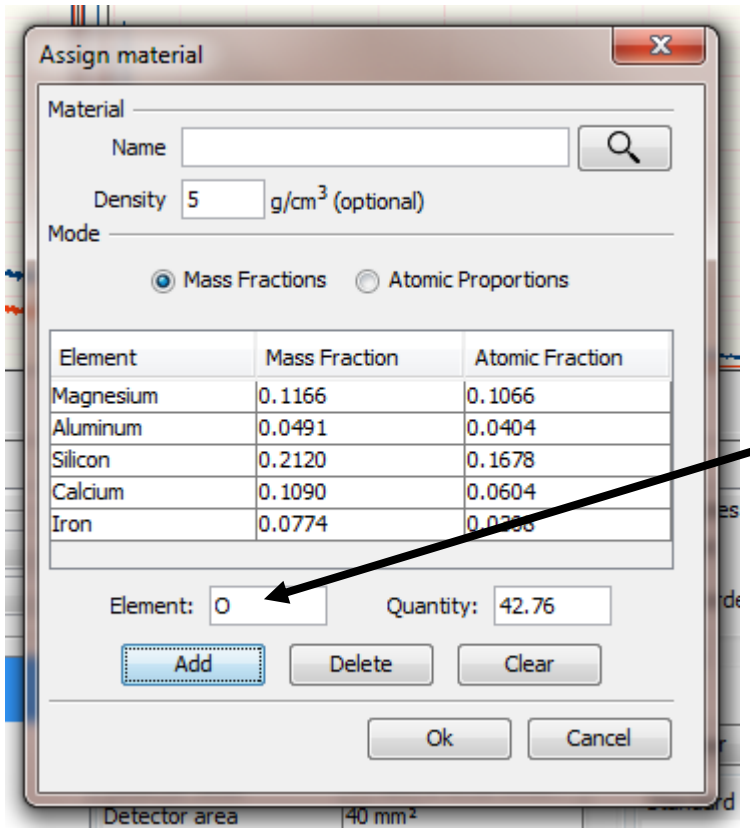
Input mode: mass fraction or atomic fraction

A table summarizing the amount of each element in the material definition.

The name, abbreviation or atomic number of the element to add.

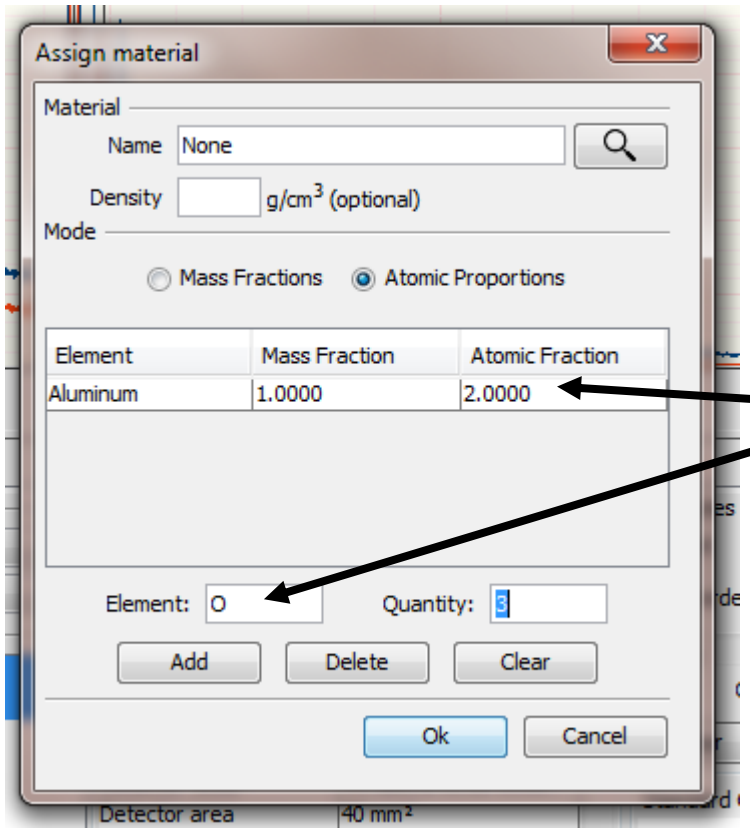
The amount to add in mass percentage or atomic fraction

Tedious – mass fraction



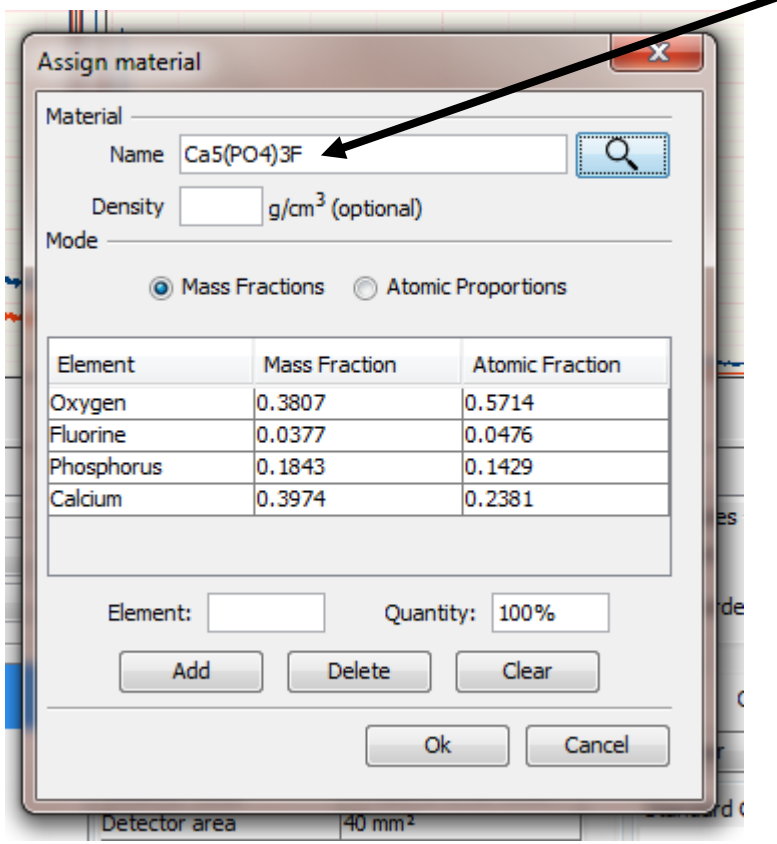
Add 0.4276 mass fraction or 42.76 mass percent O.

Tedious – mass fraction



Add 3 atoms of O per
2 atoms of O

By chemical formula



Unambiguous chemical formulas entered here are parsed and the equivalent quantity of each element is entered.

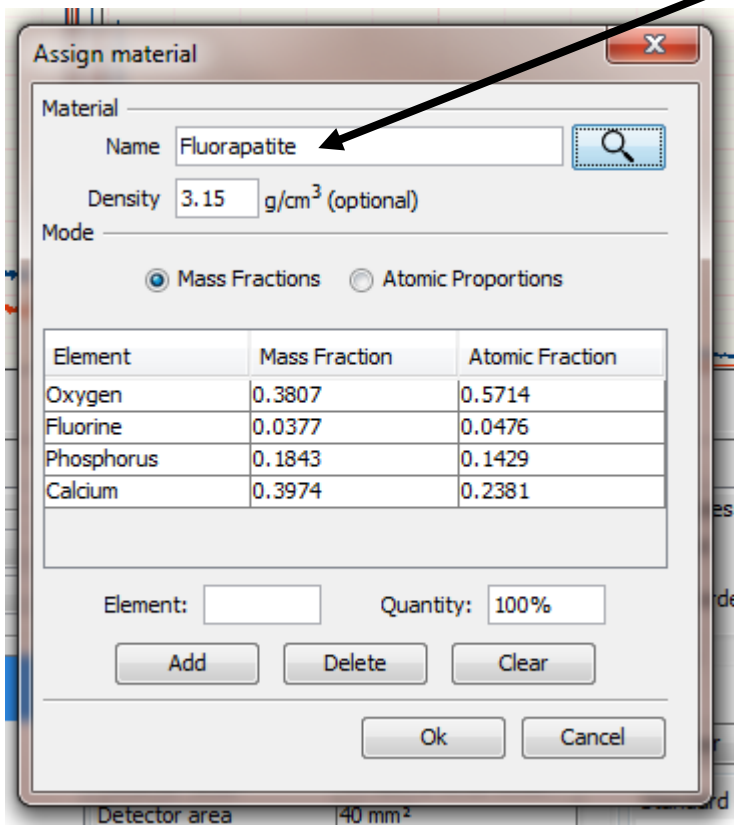
Capitalization is critical. ‘COP’ is interpreted as 1 C atom, 1 O atom and 1 P atom while ‘CoP’ is interpreted as 1 Co atom and 1 P atom. ‘CU’ is C and U while ‘Cu’ is copper.

This formula is interpreted as 5 Ca atoms, 3 P atoms, 12 O atoms and 1 F atom. The braces ‘(‘ and ‘)’ group the PO4 which is taken 3 times.

The parsing can be forced by pressing the

It is often a good idea to rename the mate after entering a parse formula. I might name this one ‘Fluorapatite’.

From the database



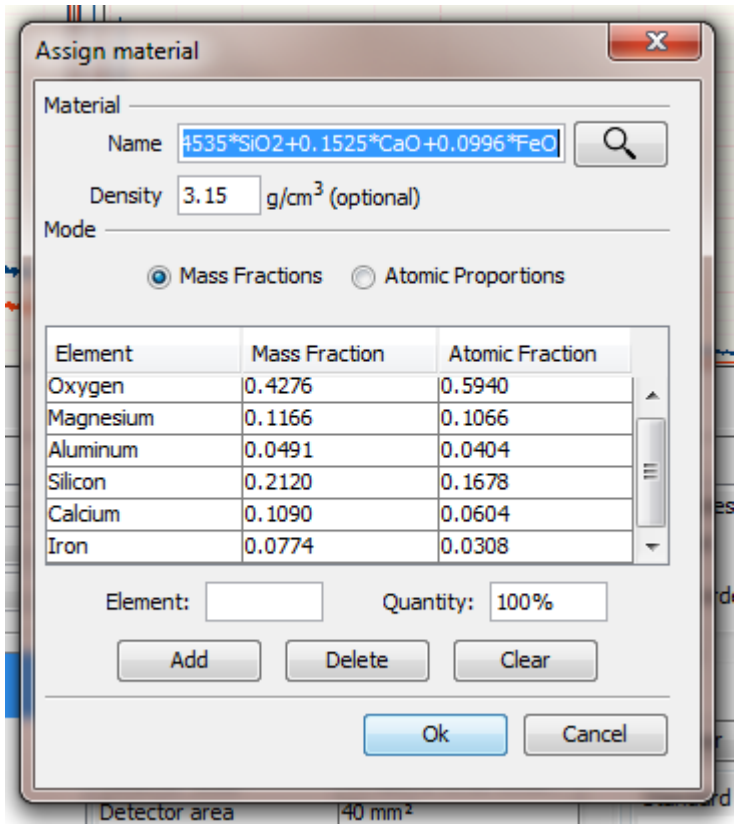
A material once entered is remembered.

DTSA-II builds a material database from the materials entered into the material editor. Whenever a name is entered into the 'Name' field, the program searches the database for previously defined materials with precisely that name. (Spelling and capitalization matter.)

The names "temp", "tmp", "crap", "junk", and "stuff" are neither stored nor retrieved.

The density is also stored in the database.

Advanced



Enter a sum of materials by mass-fraction.

For example: K412 glass is defined in terms of its oxide fractions as:

0.1933*MgO+0.0927*Al2O3+0.4535*SiO2+0.1525*CaO+0.0996*FeO

This is parsed as 0.1933 fraction by mass of MgO which is parsed as 1 atom of Mg and 1 atom of O plus 0.0927 fraction by mass of Al2O3 etc.

Remember a user-friendly name

When you click ‘Ok’, the dialog closes and the material is stored by name in the database.

If the name is easy-to-remember, you can recover the material definition from the database quickly and easily.